Optimal Heat Exchanger Rating Models for Isothermal CSTR SO3 Hydration Using Vanadium

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Abstract— *This work deals with the development of design models for heat exchanger rating in catalytic sulphur trioxide hydration process at isothermal condition exploiting the Abowei and Goodhead derived continuous adsorption tower (CAST) heat generation per unit volume equations at constant temperature. Shell and Tube heat exchanger is invoked for this studies resulting to novel design equations which were stochastically examined and found to be capable of simulating the rating performance dimensions as a function of kinetic parameters. The rating performance models were further generalized to inculcate fractional conversion functionality. The novel design models were simulation to evaluate the overall heat transfer coefficient, mass flow rate of cooling fluid, tube side cross flow area and tube side film coefficient using Matlab R2007B within the operational limits of conversion degree at constant temperature. The heat exchanger is used for the removal of heat generated per reactor unit volume utilizing water as cooling fluid, enters the shell side at 25^oC flowing counter currently to the tube side at exit temperature of 85^oC in order to maintaining 97^oC isothermal condition. The configuration of the exchanger is U–tube type and is three (3) shell and six (6) tube passes. The results of the rating dimensions showed a dependable relationship with fractional conversion at constant temperature for various reactor radius and number of tubes.*

Keywords— CAST, heat exchanger Rating, isothermal, hydration, sulphur trioxide.

I. INTRODUCTION

1.1 Stoichiometry

Catalytic hydration of sulphur trioxide using vanadium catalyst results to production of sulphuric acid and it is an industrially very important chemical specie due to its associated uses. Hence, the continuous search for the development of suitable design model to optimize its production capacity for reactor types is eminent [1]-[3]. Sulphuric acid otherwise called oil of vitrol and king of chemicals is a diprotic acid with structural formula presented in fig 1.

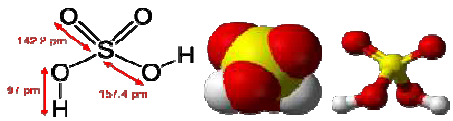

Fig.1: Sulphuric Acid Structural Profile

Sulphuric acid possesses high ionization and dissociation capacities that influence its reactivity with other chemicals resulting to useful finished industrial products with high heat of reaction that needs to be controlled using suitable heat exchanger. A heat exchanger or interchanger is a device which makes possible the transfer of heat from one fluid to another through a container wall [4]-[6]. In a typical process industry application, a heat exchanger may be a vessel in which an outgoing processed hot liquid transfers some of its heat to an incoming cold liquid about to be processed. The amount of heat so transferred is not lost to the process but, instead, is used again. Its equivalent heat need not be supplied by new fuel but may be considered as cycled heat [7]-[10]. Similarly, to maintain optimum condition for a reaction to proceed at an appreciable rate, it is imperative to control the temperature of the reaction with the aid of heat exchangers.

Although the production of sulphuric acid is eminent and known globally, related literatures have shown that numerous treaties have been written and published on it [11]. The purpose of this study is to continue investigations into past works on the development of performance models including associated heat exchangers for reactor types for the production of sulphuric acid, and to specifically identify and develop appropriate performance models for the areas that are deficient in past works. However, little or no known published work had been recorded for the development of feasible heat exchanger performance models for the production of the acid using batch, continuous stirred adsorption tower, and

plug flow adsorption towers at isothermal and non-isothermal conditions. Recently, works of Goodhead and Abowei (2014) focused on development of design models for H2SO4 production based on semi batch, isothermal plug flow (IPF) non-isothermal plug flow (NIPF) and non- isothermal continuous adsorption tower [12]

These works on the development of design models covers heat generation per unit volume for all adsorption tower types but advocated the necessity for further studies on the development of suitable heat exchanger units capable of maintaining desired temperature to obtain products in adherence to plant performance dimensions [14-[16].

Therefore, in this present paper we considered development of heat exchanger performance rating for continuous stirred tank reactor (CSTR) as a function of kinetic parameters at isothermal condition exploiting the heat generation per unit volume model of Abowei And Goodhead (2014).

1.2 KINETIC EVALUATION

The stoichiometry in the manufacture of Sulphuric Acid (H_2SO_4) is well cited in the works of Abowei and Goodhead (2014) and summarized as follows;

Combustion Chamber (combustion of sulfur) - **Converter** (conversion of sulfur dioxide) -> **Adsorption Tower** (sulfur trioxide hydration process)

The *Contact Process* is a process involving the catalytic oxidation of sulfur dioxide, SO_2, to sulphur trioxide, SO_3. A vanadium catalyst (vanadium (V) oxide) is also used in this reaction in order to speed up the rate of the reaction [12]. The current work looked at the development of performance evaluation models for vanadium catalyst based isothermal continuous stirred adsorption tower sulphur trioxide hydration process in the production of sulphuric acid. The stoichiometric chemistry is given as,

$$\left.\begin{aligned} S_{(s)} + O_{2(g)} &\rightarrow SO_{2(g)} \\ SO_{2(g)} + \tfrac{1}{2}O_{2(g)} &\longrightarrow SO_{3(g)} \\ SO_{3(g)} + H_2O_{(l)} &\rightarrow H_2SO_{4(l)} \end{aligned}\right\} \quad (1)$$

Substantial works had been done and documented on the kinetics of sulphuric acid production [9]. Literatures have shown that direct dissolution of sulphur trioxide in water to produce the acid is not done due to very high heat of reaction occasioned in the process. Instead sulphur trioxide is absorbed in concentrated sulphuric acid to form oleum, and subsequently diluted with water to form sulphuric acid of 98%-100% concentration.

The reaction mechanism as presented in equation (3) showed chain reaction characteristics reported on the photo-catalysed oxidation of SO_3^{2-} by (dimethyl-glyoximato) $(SO_3)_2^{3-}$ and its (Co(dimethyl-glyoximato) $(SO_3)^3{}_2$ [1].

The work showed that the reaction

$$SO_3 + H_2O \longrightarrow H_2SO_4 \quad (2)$$

is described as irreversible bimolecular chain reaction. Further research into the works of Erikson, [1974] established the reaction as second order reaction with rate constant K_2= 0.3 mole/sec. Blanding (1953) performed abinitio calculation and determined the energetic barrier and established conclusively that the irreversible bimolecular nature of the reaction have ΔH_r = -25kcal/mol at 25°c.

Following the outcome of the work of Chenier (1987), Charles (1997) as cited above, the rate expression for the formation and production of sulphuric acid is summarized as in equation 2.

$$-R_A = K_2 [SO_3][H_2O] \quad (3)$$

Hence from equation 3 the amount of SO_3 and H_2O that have reacted at any time t can be presented as;

$$-R_A = K_2[C_{A0} - C_{A0}X_A][C_{Bo} - C_{A0}X_A] \quad (4)$$

Where

C_{Ao} = Initial concentration of SO_3 (moles/Vol)
C_{Bo} = Initial concentration of H_2O (moles/Vol)
X_A = Fractional conversion of SO_3(%)
$-R_A$ = Rate of disappearance of SO_3 (mole/ Vol/t)

In this work, the rate expression ($-R_A$) as in equation 4 will be used to develop the hypothetical continuous stirred tank reactor tower design equations with inculcation of the absorption coefficient factor as recommended in the works of Van-Krevelen and Hoftyger cited in Austein (1984) and Danner,(1983). This is achieved by modifying equation 4 as illustrated below. The hypothetical concentration profile of the absorption of sulphur trioxide by steam (H_2O) is represented in fig.2 [1] and [17].

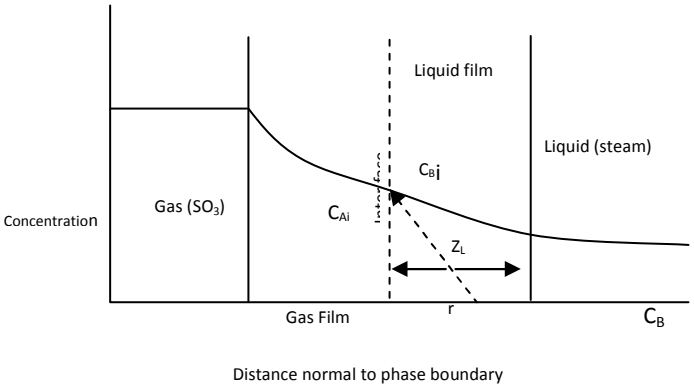

Fig.2: Absorption with chemical Reaction

trioxide (A) is absorbed into the steam (B) by diffusion. Therefore the effective rate of reaction by absorption is defined by

$$-R_A = \frac{rD_L}{Z_L}\left(C_{Ai} - C_{AL}\right) = rK_L\left(C_{Ai} - C_{AL}\right) \quad (5)$$

Invoking the works of Krevelen and Hoftyzer, the factor r is related to C_{Ai}, D_L and K_L to the concentration of steam B in the bulk liquid C_{BL} and to the second order reaction rate constant K_2 for the absorption of SO_3 in steam solution. Thus

$$r = \left(K_2 D_L C_{BL}\right)^{1/2} \Big/ K_L \quad (6)$$

Substituting equation 6 into 5 results in

$$-R_A = (C_A)\ C_{BL}^{1/2}\ K_2^{1/2}\ D_L^{1/2} \quad (7)$$

Previous reports shows the amount of SO_3 (C_A) and steam (C_{BL}) that have reacted in a bimolecular type reaction with conversion X_A is $C_{AO} X_A$ [18] and [19].

Hence equation 7 can be rewritten as

$$-R_A = K_2^{1/2} D_L^{1/2}\left(C_{BO} - C_{AO}X_A\right)^{1/2}\left(C_{A0} - C_{A0}X_A\right)$$

$$= K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2}(1 - X_A) \quad (8)$$

Where

$$m = \frac{C_{B0}}{C_{A0}}$$

m = The initial molar ratio of reactants
$-R_A$ = Rate of disappearance of SO_3
K_2 = Absorption reaction rate constant
D_L = Liquid phase diffusivity of SO_3.
K_L = Overall liquid phase mass transfer coefficient
r = Ratio of effective film thickness for absorption with chemical reaction

1.3 CSAT PERFOMANCE MODELS

Abowei and Goodhead (2014) developed CSAT performance models as

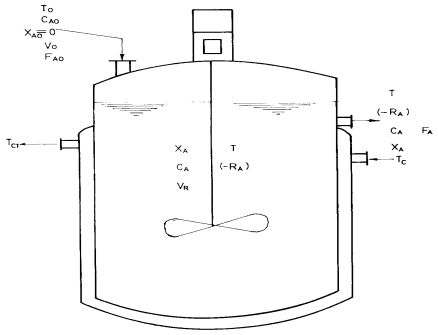

Fig.3: Hypothetical model of a Jacketed CSAT

1. 3.1 Reactor Volume

The performance equation for isothermal mixed flow reactor makes an accounting of a given component within an element of volume of the system. But since the composition is uniform throughout, the accounting may be made about the reactor as a whole [20].

Thus,

Input = Output +disappearance by reaction + accumulation (9)

Where,

Accumulation = O for steady state process.

If $F_{AO} = V_0 C_{A0}$ is the molar feed rate of SO_3 to the reactor, then considering the reactor as a whole we have

Input of SO_3, moles/time = F_{A0} (1 – X_A) = F_{A0} (10)

Output of SO_3, moles/time = F_A = F_{A0} (1 – X_A) (11)

Disappearance of SO_3 by reaction, moles/time = $(-R_A)\ V_R$ (12)

Introducing the three terms in the material balance equation (9) yields.

$$F_{A0}\ X_A = (-R_A)V_R \quad (13)$$

Which on re-arranging becomes

$$V_R = \frac{F_{Ao} X_A}{(-R_A)} \quad (14)$$

But,

$$-R_A = \frac{dC_A}{dt} = K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2}(1 - X_A)$$

Substitution in equation 14 results in

$$V_R = \frac{F_{Ao} X_A}{K_2^{1/2} D_L^{1/2} C_{AO}^{3/2} (m - X_A)^{1/2}(1 - X_A)} \quad (15)$$

F_{A0} = Molar feed rate of SO_3, (mole/sec)
X_A = Conversion degree
C_{A0} = Initial concentration of SO_3, (mole/m^3)
K_2 = Absorption reaction rate constant, (1/sec)
D_L = Liquid phase diffusivity of SO_3, (m^2 /sec)
M = Initial molar ratio of reactants.

1. 3.2 Reactor Height

Considering a reactor with cylindrical shape we have

$$V_R = \pi r^2 h$$

$$h = \frac{V_R}{\pi r^2} \quad (16)$$

$$= \frac{F_{AO}\ X_A}{\pi^2\ K_2^{1/2}\ D_L^{1/2}\ C_{AO}^{3/2}\ (m - X_A)^{1/2}\ (1 - X_A)} \quad (17)$$

For 0.1m $\leq$ r $\leq$ 1.0m

1.3.3 Heat Generation per Reactor Volume

Heat flow rate of CSAT is a function of heat of reaction for $S0_3$ addition to water, molar feed rate and the conversion degree. It is mathematically expressed as;

$$Q = (-\Delta H_R)\, F_{A0}\, X_A \qquad (19)$$

The heat generation per reactor volume is obtained by dividing both sides of equation (22) by the reactor volume and substituting equation (15) accordingly gives,

$$R_q = \frac{Q}{V_R} = (-\Delta H_R) K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2} (1 - X_A) \qquad (20)$$

From the foregoing it is obvious that the CSAT heat exchanger performance rating models are needed to control the generated per unit volume of the adsorption tower as reflected in equation (23)

There is utmost need to provide such unit for effective operation of the plant to enhance productivity. Hence, this study is focused appraise series of shell-and-tube heat exchanger to solve the problem of heat effect involved in SO_3 hydration for the CSAT plant.

II. MATERIALS AND METHODS

2.1 Development of Models

In this heat exchanger the product (H_2SO_4) flows through the tube side while the cooling fluid (water) passes through the shell side counter currently. Shell-and-tube heat exchangers are used commonly in industries and aimed at maintaining constant temperature for the production of sulphuric acid. Therefore highlighted herein is development of heat exchange rating models in evaluating overall heat transfer coefficient, heat transfer surface (area), tube numbers per shell, mass flow rate of cooling fluid, tube-side film coefficient, shell side film coefficient using the models as developed from equations (1) to (23) of this work. The diagram in fig. 1 shows the configuration of the CSAT with the proposed shell-and-tube heat exchanger for the study.

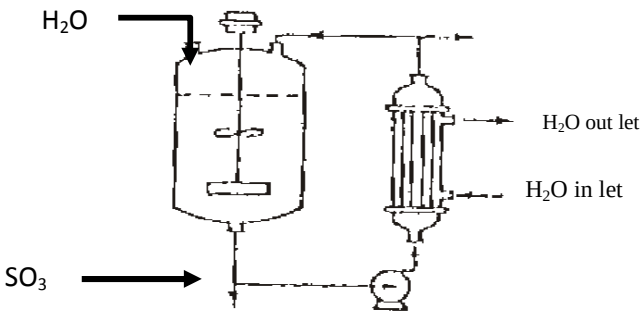

Fig.4: Hypothetical heat exchanger rating unit.

2.1.1 Overall Heat Transfer Coefficient (OHTC)

The design equation for OHTC is usually obtained from the heat generation per unit volume of the reaction tower as in equation (20) [21] and [22].

Thus,

$$R_q = UA\Delta T_m \qquad (21)$$

Equations (17), (20) and (21) could be compared resulting in the design equation for the computation of OHTC as a function of kinetic parameters;

$$R_q = \frac{Q}{V_R} = \frac{\frac{-\Delta H_r F_{A0} X_A}{F_{A0} X_{A0}}}{\pi r^2 K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} (M - X_A)^{1/2} (1 - X_A)} \qquad (22)$$

And equation (22) subsequently simplified to gives;

$$UA\Delta T_m = -\Delta H_r \pi r^2 K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} (M - X_A)^{1/2} (1 - X_A)$$

$$U = \frac{-\Delta H r\, \pi r^2 K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} (M - X_A)^{1/2} (1 - X_A)}{A\Delta T_m} \qquad (23)$$

2.1.2 Mass Flow rate of Cooling Fluid

In order to functionalized mass flow rate dependency on total amount of heat generated per reaction tower volume, and recalling that;

$$R_q = \frac{Q}{V_R} = G.C_p\, \Delta T_m \qquad (24)$$

Where G = Mass flow rate of cooling fluid
C_p = Heat capacity
ΔT = Temperature

Mass flow could be computed by equating equations (24) and (22) thus;

$$UA\Delta T_m = -\Delta H_r \pi r^2 K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} (M - X_A)^{1/2} (1 - X_A) \qquad G = \frac{-\Delta H_r \pi r^2 K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} (M - X_A)^{1/2} (1 - X_A)}{C_p\, \Delta T_m} \qquad (25)$$

Where ΔT_m is calculated from Logarithmic Mean Temperature Difference (LMTD) as

$$\text{LMTD} = \frac{(T_1 - t_1) - (T_2 - t_2)}{In \dfrac{(T_1 - t_1)}{(T_2 - t_2)}} \qquad (26)$$

And further correlated;

$$\Delta T_m = (\text{LMTD}) * F \qquad (27)$$

Where F is a correction factor usually obtain from charts. To read the charts values for P and R (temperature coefficients) are calculated using the following expressions.

$$P = \frac{t_2 - t_1}{T_1 - t_1} \quad and \quad R = \frac{T_1 - T_2}{t_2 - t_1} \qquad (28)$$

2.1.3 Tube-Side models

(a) Tube Side Cross Flow Area

The tube side cross flow area is also correlated to reaction tower height for effective control of heat throughput and calculated from;

$$a_t = \frac{\pi DiL}{n} \qquad (29)$$

Interestingly, kinetics parameters were invoked by substituting equation (17) into (29) to giving;

$$a_t = \frac{\pi D_i F_{A0} X_A}{n\pi r^2 K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} (M-X_A)^{1/2} (1-X_A)} \quad (30)$$

Where a_t = tube side cross flow area

n = number of tube passes

L ⇒ H = Height of reactor tower

2.1.4 Tube side mass velocity model

The tube side mass velocity, G_t is given by

$$G_t = \frac{G}{a_t} \quad (31)$$

Putting

$$\alpha = \pi r^2 K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} \quad (32)$$

Then, mass flow rate (G);

$$G = -\Delta H_r \alpha (M - X_A)^{1/2} (1 - X_A) \quad (33)$$

And

$$a_t = \frac{\pi D_i F_{A0} X_A}{n \alpha (M-X_A)^{1/2} (1-X_A)} \quad (34)$$

Substituting equations (33) and (34) into (31) results;

$$G_t = \left[\frac{-\Delta Hr\, \alpha (M-X_A)^{1/2} (1-X_A)}{\pi D_i F_{A0} X_A}\right] \left[n \alpha (M - X_A)^{1/2} (1 - X_A)\right] \quad (35)$$

Equation (35) further be summary to give;

$$G_t = \frac{-\Delta Hr\, \alpha^2 [(M-X_A)(1-X_A)]^2 n}{\pi D_i F_{A0} X_A} \quad (36)$$

III. PERFORMANCE RATING DESIGN CALCULATION

Basic design calculation for the performance rating was well evaluated using all the model equations in (13) to (30). These design calculations are summarized as

A. Tube-Side Film Coefficient

The fundamental equation for turbulent heat transfer inside tubes in given by perry and green (1997). [25]

$$Nu = 0.027 (Re)^{0.8} (Pr)^{0.33} \quad (37)$$

Or

$$\frac{h_i D_i}{K_W} = 0.027 \left(\frac{D_i G_t}{\mu_W}\right)^{0.8} \left(\frac{C_{pW} \mu_W}{K_W}\right)^{0.33} \quad (38)$$

From equation 33, it was possible that,

$$h_i = 0.027 \frac{K_w}{D_i} \left(\frac{D_i G_t}{\mu_w}\right)^{0.8} \left(\frac{Cp_w \mu_w}{K_w}\right)^{0.33} \quad (39)$$

Where h_i is the tube side film coefficient

3.2 INTERNAL DIAMETER OF SHELL

The internal diameter of the shell can be calculated using Reynold's number (Re). when the Reynolds number is less than 2100 we have a laminar flow but if the Reynolds's number is between 2100 and 10,000 then it is in the transition regime. For turbulent flow of viscous fluids the Reynold's number is greater than 10,000. For a baffled shell-and –tube exchanger, the turbulent regime is preferred because it gives high heat transfer rates [21].

Taking Re = 10,100

$$Re = \frac{DG}{\mu} = 10{,}100 \quad (40)$$

$$D = \frac{Re\ \mu}{G} \quad (41)$$

Where D – internal diameter of shell

Let a_s be the shell-side cross flow area, then

$$a_s = \frac{D * C_t * B}{P_t} \quad (42)$$

Where B - Baffle spacing = 1/5 (D)

For three shell passes, equation (37) is modified, Perry& Green(1997) as

$$a_s = \frac{1}{3} \frac{(D * C_t * B)}{P_t} \quad (43)$$

3.3 SHELL-SIDE MASS VELOCITY

Let G_s be the shell side mass velocity, then

$$G_s = \frac{G_0}{a_s} \quad (44)$$

The shell side equivalent diameter, De is given by

$$De = \frac{4\left(P_t^2 - \pi / 4 D_0^2\right)}{\pi D_0} \quad (45)$$

3.4 SHELL-SIDE FILM COEFFICIENT

According to the Donohue equation, turbulent heat transfer outside the tubes of a segmental baffled heat exchanger is given by; [21]

$$Nu = \frac{a_0}{F_s} (R_e)^{0.6} (P_r)^{0.33} \quad (46)$$

For tubes staggered in the tube bundles

$$a_0 = 0.33 \ and \ F_s = 1.6$$

Then equation (18) is written as

$$\frac{h_0 D_e}{K_0} = 0.21 \left(\frac{D_e G_s}{\mu_0}\right)^{0.6} \left(\frac{C_{po} \mu_0}{K_0}\right)^{0.33} \quad (47)$$

3.5 FLUIDS PROPERTIES FOR SIMULATION

The heat exchanger model equations developed in section 2.0 contain unknown physical parameters such as the density, viscosity, specific heat capacity, thermal conductivity of the fluids. These physical parameters have to be determined before equations (1) – (25) can be evaluated. The operating conditions and physical properties of the fluids specific for the heat exchanger are presented in Table 1 and 2.

Table 1: Physical properties of Water

Physical Properties	**Values**
Mass flow rate, G_w	1.334 Kg/Sec
Inlet temperature, T_1	25°C
Outlet temperature, T_2	85°C

Average temperature, T_{av}	55°C
Specific heat capacity at 55°C, C_{Pw}	4.2KJ/Kg K
Thermal Conductivity at 55°C, K_w	0.6W/mK
Fouling Resistance at 55°C, F_s	0.00005K.m^2/W
Viscosity at 55°C, μ_w	5.0x10^{-4}Kg/ ms

Table 2: Physical properties of Sulphuric acid

Physical Properties	**Values**
Mass flow rate, G_p	0.3858 Kg/Sec
Inlet temperature, t_1	95°C
Outlet temperature, t_2	97°C
Average temperature, t_{av}	96°C
Specific heat capacity at 96°C, C_{Pa}	1.38KJ/Kg K
Thermal Conductivity at 96°C, K_a	0.25W/mK
Fouling Resistance at 96°C, F_t	0.003K.m^2/W
Viscosity at 96°C, μ_a	5.0x10^{-3}Kg/ms

3.6 TUBE SPECIFICATION

The heat exchanger tube dimensions, tube clearance, and tube pattern as obtained in Perry chemical engineer's handbook are presented in Table 3.The standard tube dimension chosen is ¾" by 20ft.

Table 3: Tube Specification

Property	**Dimension**
Outside diameter of tube, DO	19.05mm
Thickness of tube, XW	2.11mm
Internal diameter of tube, Di	14.83mm
Tube clearance, Ct	5.95mm
Tube pitch, Pt	25.0mm
Length of tube, L	6.10m (or 20ft)
Tube pattern	Square

IV. COMPUTATIONAL FLOW CHART

The computation of the functional parameters of the heat exchanger as shown in fig.1 is implemented in MATLAB, and the computer flow chart describing the computation is illustrated in fig 5.

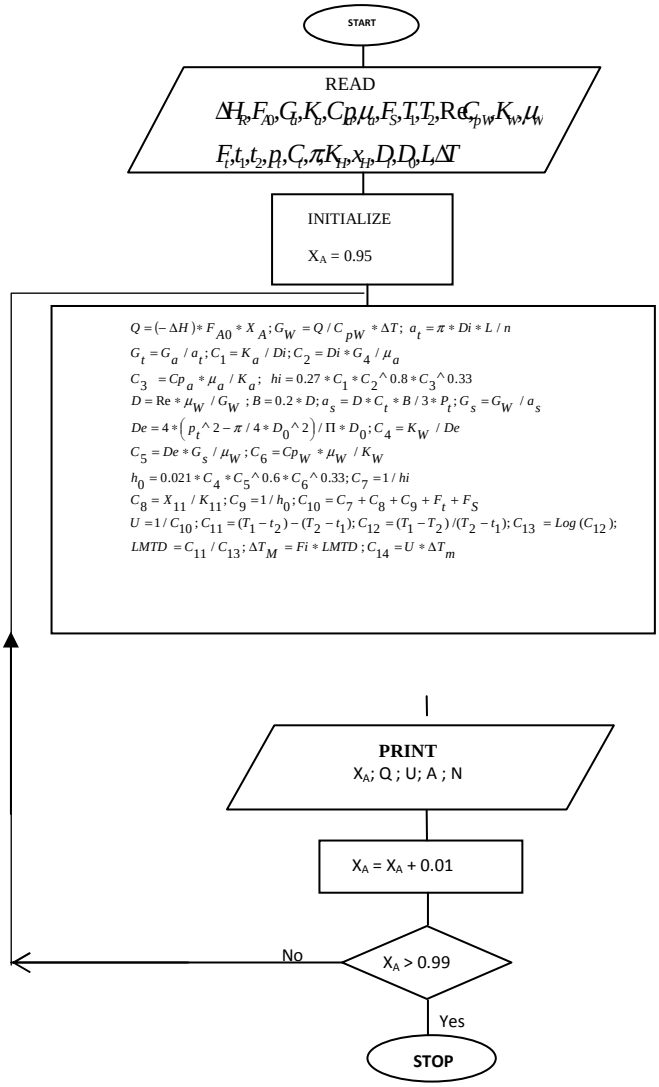

Fig.5: Flow Chart Describing the computation of functional parameters of Isothermal CSTR heat exchanger Unit.

V. RESULTS AND DISCUSSION

Model equations as developed in equations (23) to (35) were simulated using matlab 2014b for overall heat transfer coefficient, mass flow rate of cooling fluid, tube site flow area and tube side mass flow velocity exploiting the kinetic parameters. The results obtained are presented and discussed below.

5.1 OVERALL HEAT TRANSFER COEFFICIENT

Fig. 6 give results of overhead heat transfer coefficient as a function of fractional conversion for various CSAT radius.

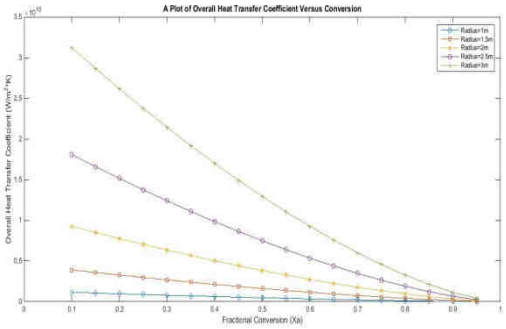

Fig.6: overall heat transfer coefficient vs conversion

The results shows that overall heat transfer coefficient decreases with increase in fractional conversion and the plot demonstrated non-linearity with characteristics slope(S_u) defined as;

$$S_U = \frac{-\Delta Hr\pi\, K_2^{1/2}\, D_L^{1/2}\, C_{A0}^{3/2}}{A\Delta T_m} \qquad (48)$$

Therefore, a novel model to predict overall heat transfer coefficient can be summarized in equation (48), thus;

$$U = S_u\,(M - X_A)^{1/2}(1 - X_A) \qquad (49)$$

5.2 MASS FLOW RATE OF COOLING FLUID

Result of mass flow rate of cooling fluid as a function of conversion for various CSAT radius and heat exchanger number of tubes are presented in fig. 7.

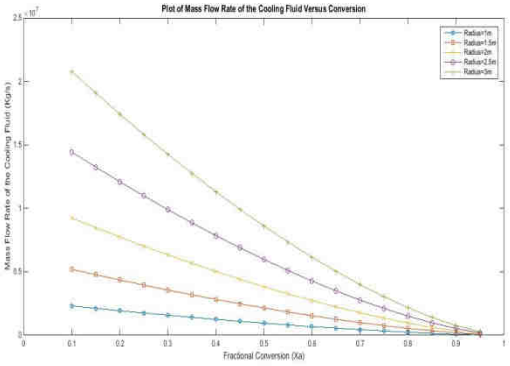

Fig.7: Mass Flow Rate of Cooling Fluid versus Fractional conversion

The results as presented in fig.7 show that mass flow rate of cooling fluid of the heat exchanger decrease with fractional conversion for various CSAT radius. A slope (S_m) describing the characteristic behavior of non-linearity is given as;

$$S_m = \frac{-\Delta Hr\,\pi r^2\, K_2^{1/2}\, D_L^{1/2}\, C_{A0}^{3/2}}{C_P\,\Delta T_m} \qquad (50)$$

Now, we substituted the slope as in equation (50) into (25) gives a summarized mass flow rate of cooling fluid predictive model as a function fractional conversion for a typical isothermal CSAT heat exchanger unit; thus

$$G = S_m\,(M - X_A)^{1/2}\,(1 - X_A) \qquad (51)$$

5.3 TUBE SIDE CROSS FLOW AREA

Simulation was carried out to study the parametric behavior of kinetics data particularly fractional conversion dependency on tube side cross-flow area of heat exchanger. The results obtain are well presented in figure 8 for various CSAT radius and tube side numbers.

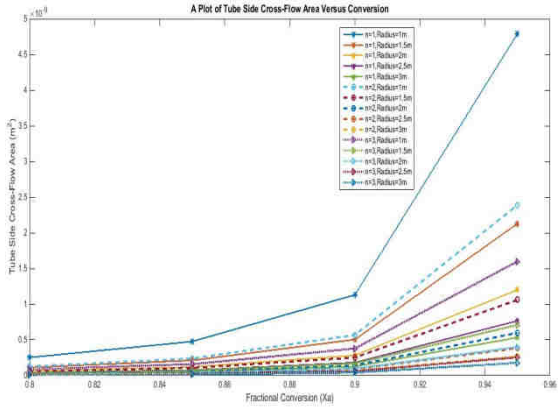

Fig.8: Tube side cross-flow area versus fractional conversion

The results as reflected in fig. 8 show great dependency of heat exchanger tube side cross-flow area as a function of isothermal CSAT fractional conversion for various radius and tube numbers. Increase in heat exchanger tube side cross-flow area increases CSAT fractional conversion at constant temperature. The slope (S_a), which demonstrate non-linearity, describing his characteristic behavior is given as;

$$S_a = \frac{\pi D_i\, F_{A0}}{n\,\pi r^2\, K_2^{1/2}\, D_L^{1/2}\, C_{A0}^{3/2}} \qquad (52)$$

Therefore simplified model for the simulation of heat exchanger tube side cross-flow area as a function of CSAT fractional conversion at constant temperature was obtain by substituting equation (51) into (30), giving;

$$a_t = \frac{S_a\, X_A}{(M - X_A)^{1/2}\,(1 - X_A)} \qquad (53)$$

5.4 TUBE SIDE MASS FLOW VELOCITY

Computation is made for heat exchanger mass flow rate as a function of CAST fractional conversion for various radius and tube side numbers, and results obtained are presented in figure 9.

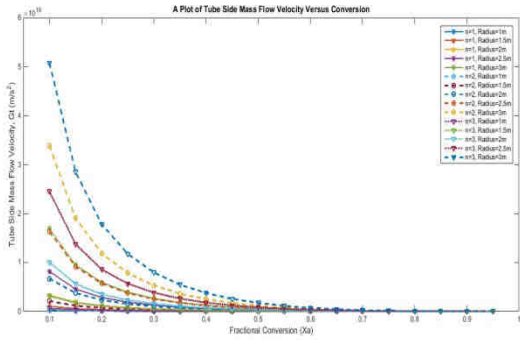

Fig.9: Tube Side Mass flow Velocity versus fractional conversion

The results as reflected in fig. 9 demonstrated tube side mass flow velocity dependency on CSAT fractional conversion at constant temperature for various radius and number of tubes. Increase in tube side mass flow velocity of the heat exchanger decreases fractional conversion. The behavior is more pronounced at 50% conversion signifying optimal operational limit of the hydration process of sulphur trioxide. The slope (S_{tv}) of the graphs was deduced resulting in;

$$S_{tv} = \frac{-\Delta Hr\ \alpha^2 n}{\pi D_i F_{A0}} \qquad (54)$$

Equations (54) and (36) were compared in order to provide a summarized predictive model of heat exchanger tube side mass flow velocity as function of CSAT fractional conversion at temperature, thus;

$$G_t = S_{tv}\ [(M - X_A)\ (1 - X_A)^2]X_A^{-1} \qquad (55)$$

Interestingly, the simulated results were captured to reflect the realities of the CSAT heat exchanger unit at isothermal condition and are summarized in table 4. The as presented for the designed heat exchanger unit are primarily to ensure removal of the heat of reaction in the reactor at isothermal condition.

Table 4: Summary of the designed heat exchanger

S/N	Parameter	Shell-side	Tube-side
1	Fluid Material	Water	Sulphuric acid
2	Flow rate (Kg/hr)	1.334	0.3858
3	Inlet temperature (^oC)	25	95
4	Out let temperature (^oC)	85	97
5	Fouling ($K.m^2/W$)	0.00005	0.003
6	Type		U – tube
7	Service		To maintain isothermal condition
8	Overall heat transfer coefficient (W/m^2K)		62.714
9	Heat duty (KJ/sec)		342.9914
10	LMTD (^oC)		31.4
11	Surface Area (m^2)		170.66m^2
12	Shell internal diameter (m)		3.79
13	Number of Shells		3.0
14	Type of Arrangement		Series
15	Baffle type		Segmental
16	Baffle spacing (mm)		200
17	Number of tubes per shell		175
18	Tube length (m)		6.1
19	Tube outside diameter (mm)		19.05
20	Tube pitch (mm)		25
21	Tube pattern		Square
22	Material of construction		Hastelloy

VI. CONCLUSION

Novel models were developed to design heat exchanger to control the heat generated per unit volume in a continuous stirred tank reactor at constant temperature for the production of sulphuric acid. The heat exchanger rating models were developed and generalized from theoretical consideration and capable of predicting sulphuric plant dimensions under isothermal condition.

The matlab based simulated results shows that overall heat transfer coefficient mass flow rate of cooling fluid, tube side mass flow velocity decreases with increase in fractional conversion and the plots demonstrated non-linearity. Similarly, Increase in heat exchanger tube side cross-flow area increases fractional conversion at constant temperature. The behavior is more pronounced at 50% conversion signifying optimal operational limit for sulphur trioxide hydration process.

In addition, the analogy as presented above portrayed compatibility of the results simulated for overall heat transfer area, mass flow rate of cooling fluid, tube side cross flow area and tube side mass flow velocity as function of kinetic parameters at isothermal condition.

NOMENCLATURE

A, total heat transfer area
A_t, area of one tube
a_s, shell side cross flow area
a_t, tube side cross flow area
B, baffle spacing
C_{Pa}, specific heat capacity of sulphuric acid
C_{Pw}, specific heat capacity of water
C_t, tube clearance
D, internal diameter of shell
D_e, shell side equivalent diameter
D_i, internal diameter of tube
D_m, mean diameter of tube
D_O, outside diameter of tube
F_t, mean temperature difference correction factor

F_s, fouling resistance
G, mass flow rate
G_a, mass flow rate of sulphuric acid
G_w, mass flow rate of water
G_S, shell side mass velocity
G_t, tube side mass velocity
hi, inside film transfer coefficient
h_O, outside film transfer coefficient
K_a, thermal conductivity of sulphuric acid
K_w, thermal conductivity of water
K_H, thermal conductivity of hastelloy
L, Length of tube
LMTD, logarithmic mean temperature difference
N, total number of tubes
n, number of tube passes
P, temperature efficiency
P_t, tube pitch
Q, quantity of heat transferred per unit time
R, temperature correction index
ΔT, temperature difference
ΔT_m, mean temperature difference
t_1, inlet temperature of sulphuric acid
t_2, outlet temperature of sulphuric acid
T_1, inlet temperature of water
T_2, outlet temperature of water
U, overall heat transfer coefficient
X_W, thickness of tube

Greek Letters

μ_w, viscosity of water
μ_a, viscosity of sulphuric acid

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